

# Linking Diffusion Map variables with equation-free multiscale computations

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Developing effective descriptions of the microscopic dynamics of many physical phenomena can both dramatically enhance their computational exploration and lead to a more fundamental understanding of the underlying physics. Obtaining a good set of variables (macroscopic observables) becomes an important step of such a modeling task.

We will illustrate this through the problem of a driven interface in the presence of mobile impurities, for which an effective reduced model was previously developed based on an Ising variant model and a single empirical coarse variable. The model was partially successful, yet it underlined the necessity of selecting additional coarse variables in certain parameter regimes.

We now use a data mining approach to help identify the coarse variables required.

We discuss the implementation of this Diffusion Map approach, the selection of a similarity measure between system snapshots required in the approach, and the correspondence between empirically selected and automatically detected coarse variables.

We conclude by illustrating the use of the diffusion map variables in assisting the atomistic simulations, and we discuss the translation of information between fine and coarse descriptions using lifting and restriction operators.